Transformative Theory and Predictive Modeling
-- a pathway toward fusion energy

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List of Contributors

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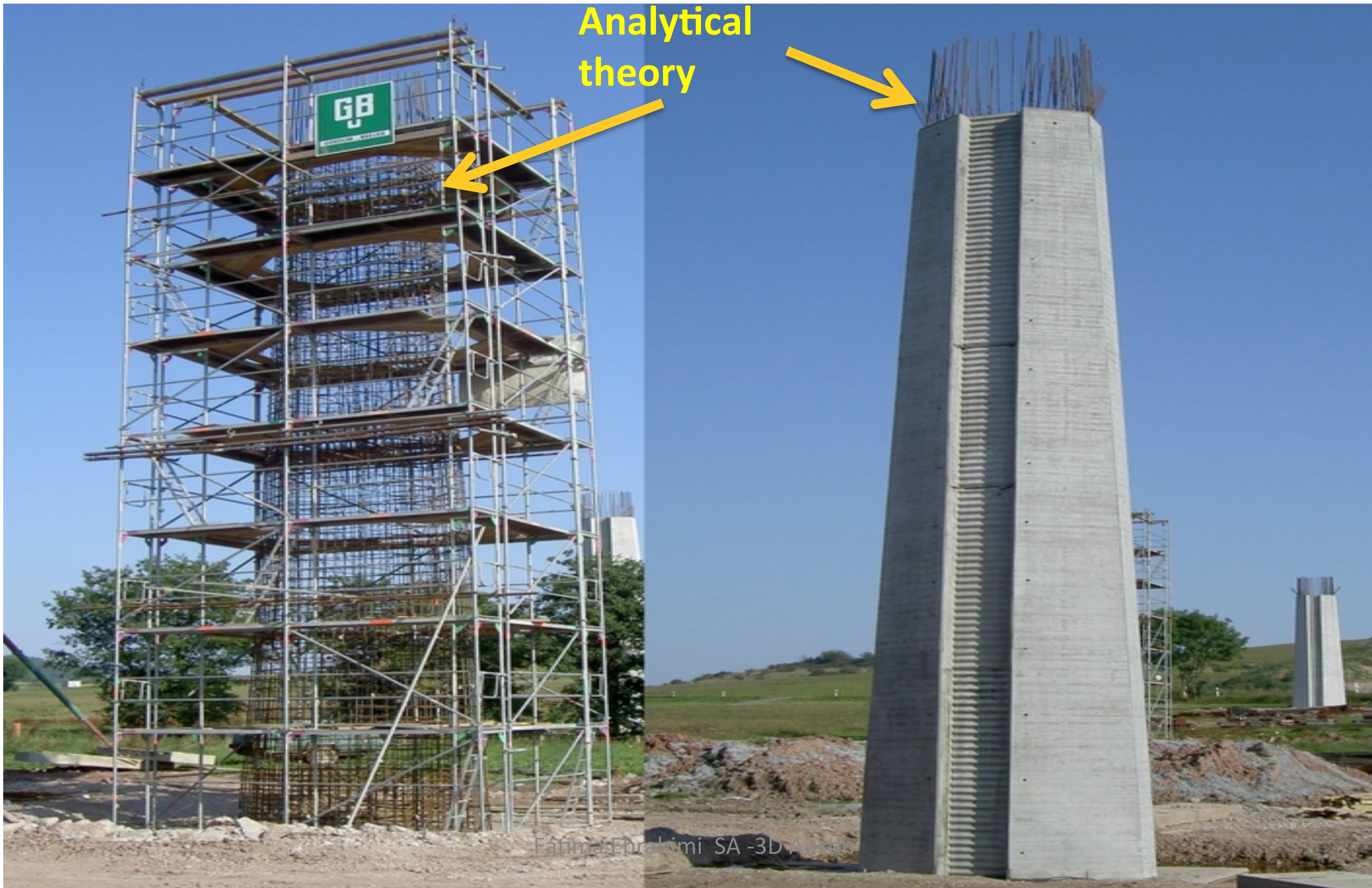
- **What do we mean by transformations**?

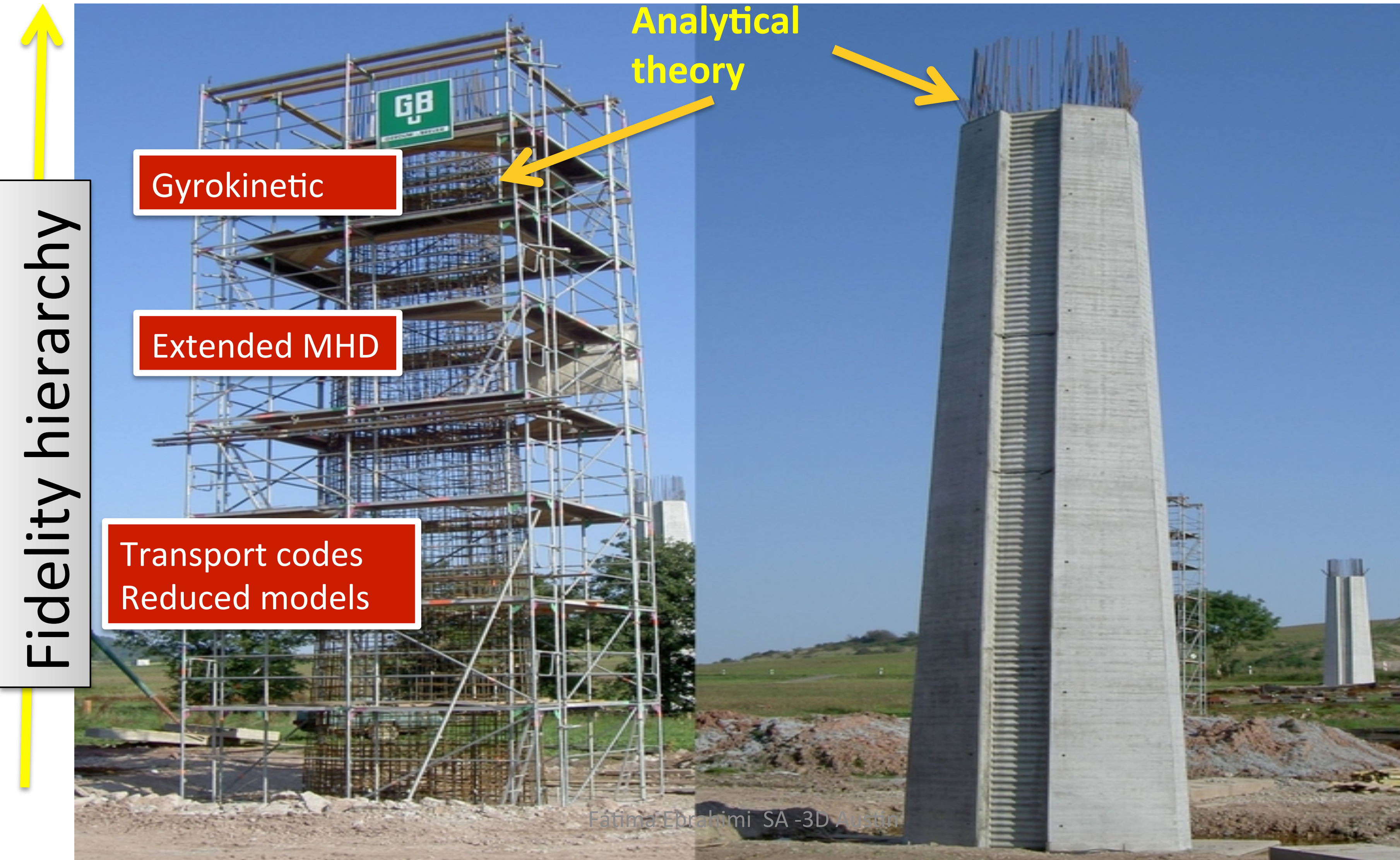
  - Breakthrough/transformation through predictive computing for "optimization of existing concepts" or "new concepts"

  - Large improvements to the existing computational techniques and models to close the existing gaps for reliable prediction for burning plasmas

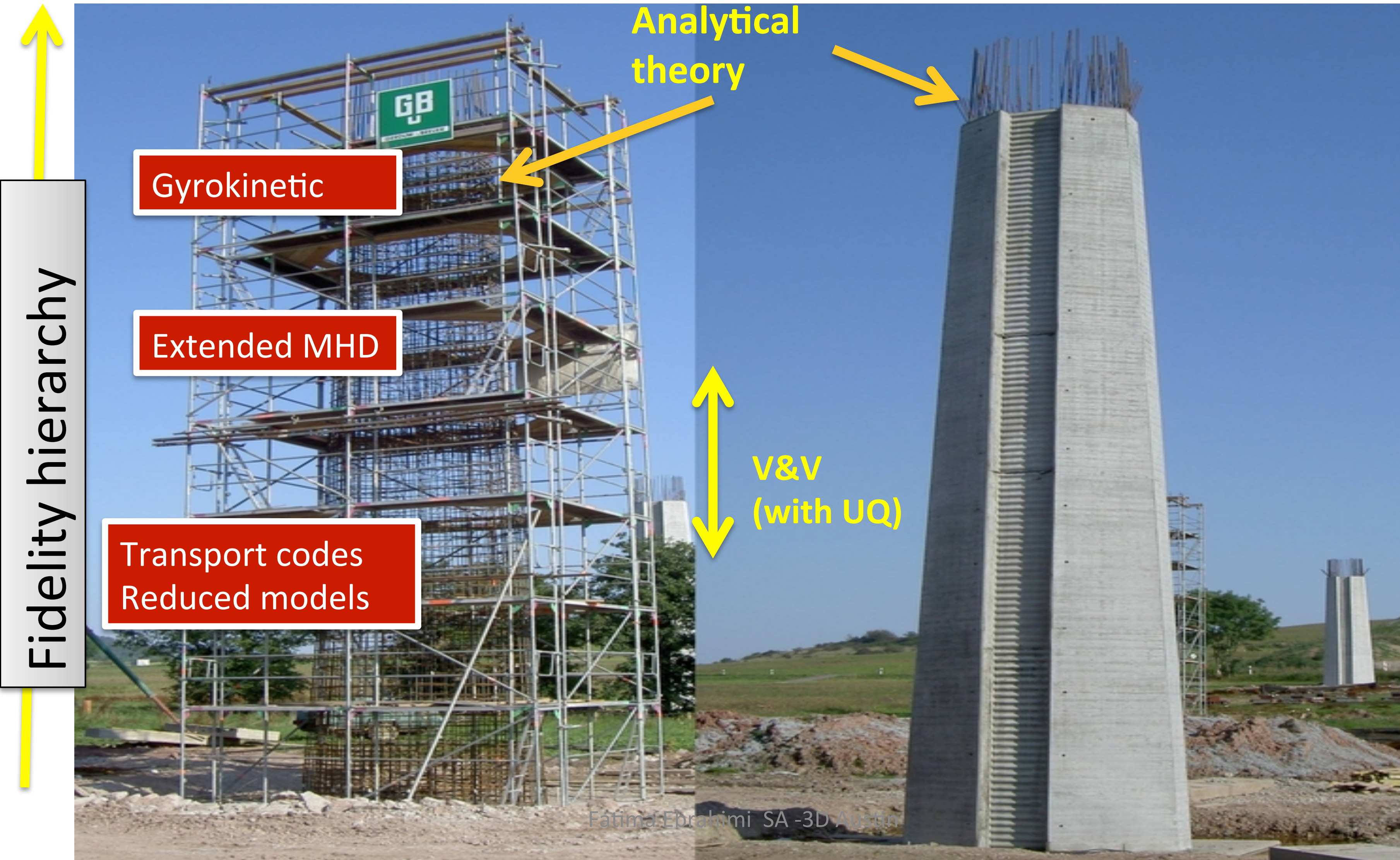
Concrete needs to be reinforced by rebar, Computation needs to be reinforced by theory



Multiphysics - Multiscale
High fidelity to reduced models needed



V&V (including experiments via synthetic diagnostic) is required at every level



The ultimate goal is to achieve optimization/prediction/control for burning plasmas through WDM

In red:
Challenging
In green:
Advantages

Whole device modeling (WDM)

1- Standalone models

- **Fluid: scale-limited but useful for disruption/ macroscopic behavior**
- **First principle kinetic: Scale-sufficient but needs extreme computing powers**

2- Reduced models (transport, Edge-models)

Between shots interactive capacity computing
Reduced fidelity

3- Integrated modeling through multiphysics-multiscale coupling
Extensive applied math/computer science effort but Scale-sufficient/fast on exascale

Challenges for high-fidelity Whole Device Modeling

- **Implicit time-advance (bridging time-scales)**
- **Large spans of temporal and spatial scales**
  - Steep gradients (edge), large range of timescales
  - require high order spatial/temporal algorithms
- **Continuity of solutions across separatrix**
- **Noise-reduction techniques**
- **Input uncertainties**
  - Verification, validation with UQ
- **Synthetic diagnostics and data management**

> - **Mathematical and computational technologies will be needed**
> - WDM = Fusion + Computer science +Applied Math
> - **Inclusion of advanced solver/iteration algorithms**

List of Innovations from SA-3 spreadsheet in different areas

	Fusion pathways->	Configurations		Technology		Understanding
Fusion Energy Objectives		Optimized stellarator (QH, QA, QO)	Advanced/ Compact/ Spherical tokamak	Plasma Technology	Fusion Nuclear Technology	Theory and Modeling
Improved plasma science	Confinement with Confidence					
	Plasma Transients Controlled					
	Maintain Burning Plasma					
Improved device performance	Higher field, pressure operation					
	Steady state operation					
Materials	Plasma Material Interaction					
	Lower Activation w/ long life					
Sustaining the fuel cycle safely	Safe Self Sufficient Tritium Systems					
	Siting and Operating D/T Facilities					

Summary list of innovations:

Improved plasma science → Predictive integrated modeling

- Exascale computing: high fidelity integrated modeling
- GPU (graphical processor unit) computing
  - integral part of leadership class computers
- Applications of advanced numerical algorithms
- Deep learning, artificial intelligence

Improved device performance → Design optimization

- Development of a predictive capability for non-inductive current-drive techniques (helicity injection, RF), and RF edge interactions
- Improved Stellarator optimization
- Integrated Physics and Engineering design

Plasma material interaction

- Reliably predict scrape-off layer transport and beyond

Prediction, avoidance, detection and mitigation of <u>transient events</u>

- Objective: Prediction/detection of transient events (disruptions, ELMs, etc.)

➢ **Innovations:**

  - **New understanding/prediction of structure and evolution of coupled pedestal/ SOL system through 3D MHD/two-fluid codes for ELM growth and ejection, coupling to electromagnetic gyrokinetic simulations**
  - **Modeled (synthetic) sensors to detect/ understand physics of event triggering**
  - **Universal predictors (e.g. machine learning) , experimentally validated reduced models to condense full physics models**
  - **Direct measurement of stability and wall responses (MHD spectroscopy, Surface diagnostics for material flaking/droplet detection, etc.)**

Prediction, avoidance, detection and mitigation of transient events

- Objective: Avoidance of transient events

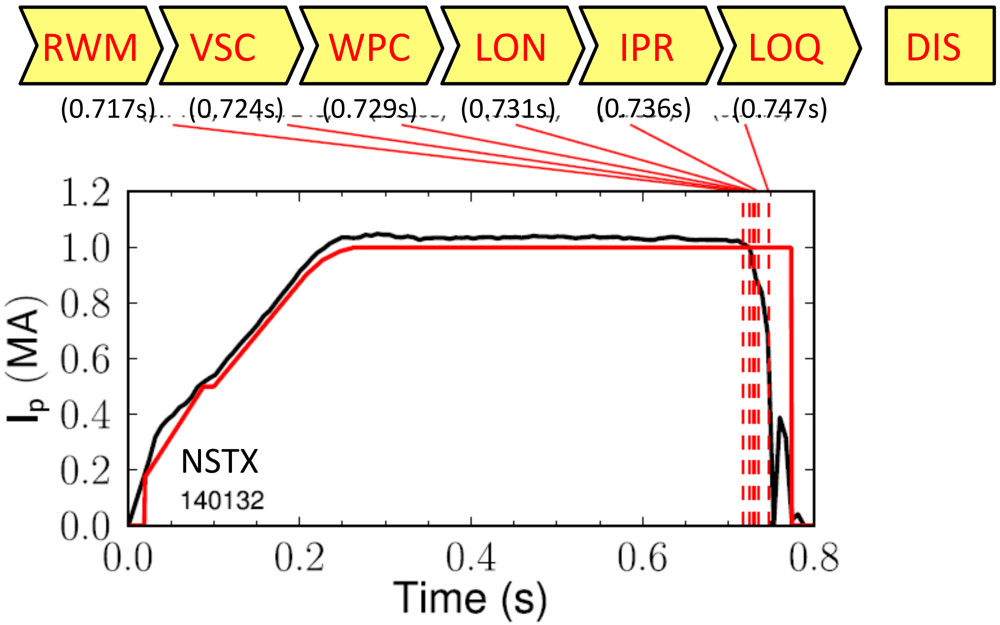
➢ **Innovations:**
  - **Elevated q operation, passive stabilization at high beta (e.g. kinetic effects) leveraged by Compact/ST design, higher B_T (e.g. use of HTS magnets)**
  - **Use of 3D fields, RF, compact torus injection for generation of plasma rotation**
  - **Real-time (r/t) disruption forecasting from theory-based stability maps**
  - **Real-time physics-based plasma profile and instability control/modeling (e.g. rotation and current profile control w/ NBI, NTV, RF; r/t predictive transport)**
  - **Resilient, replenishable first wall solutions (e.g. liquid metal, flowing powder)**

- Objective: Mitigation of transient events

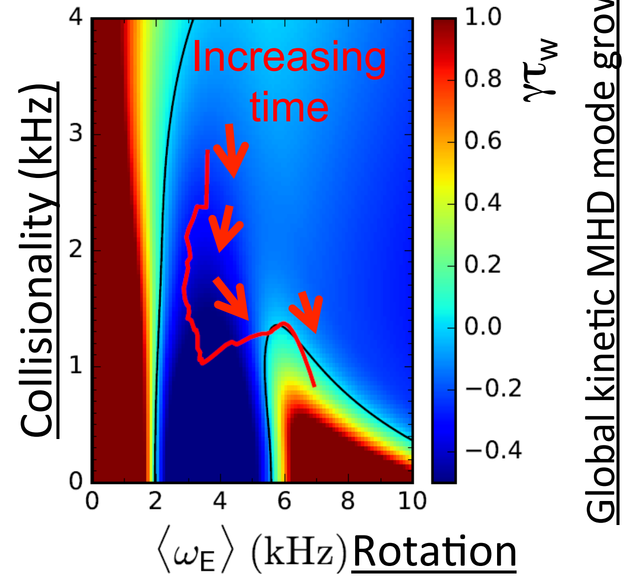
➢ **Innovations:**
  - **Core plasma mitigation solution (e.g. shell pellet, two-stage gas gun)**
  - **High-speed mitigation solution (e.g. EM injector, compact torus (CT) injection)**
  - **Self-consistent validated modeling of mitigation techniques**

Disruption Event Characterization and Forecasting innovation to enable disruption avoidance

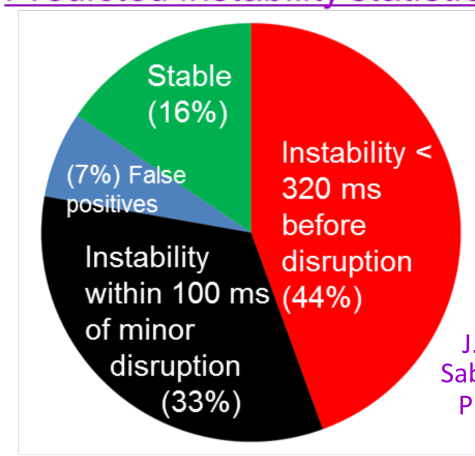
Automated disruption event chain analysis



Disruption forecasting



Predicted instability statistics



J.W. Berkery, S.A. Sabbagh, et al., Phys. Plasmas **24** (2017) 056103

Cue disruption avoidance systems

- Physics-based disruption forecasting
- Prediction quantitatively compared to experiment
- Collaborative (inter)national multi-device studies

DECAF code

Integrated steady-state higher-performance burning plasmas from core to edge

- Objectives: Full potential and viability of non-inductive techniques (solenoid-free helicity injection, RF, neutral beam)

➢ **Innovations:**

- **Validated predictive extended MHD simulations for non-inductive solenoid-free helicity injection current-drive techniques should be integrated from the edge to the core, and show that current and heat could be built up in the plasma core and form a steady state.**

- Objectives: Understanding how RF launching structures and antennas launch waves through the edge into the core

➢ **Innovations: Development of a predictive capability for self-consistent interaction of RF power with the scrape off layer and wall, including realistic antenna and first wall geometry, will provide a tool that as yet does not exist to mitigate and minimize RF power losses in the boundary plasma. Modeling to investigate high-field LHCD launch and its impact on the microturbulence.**

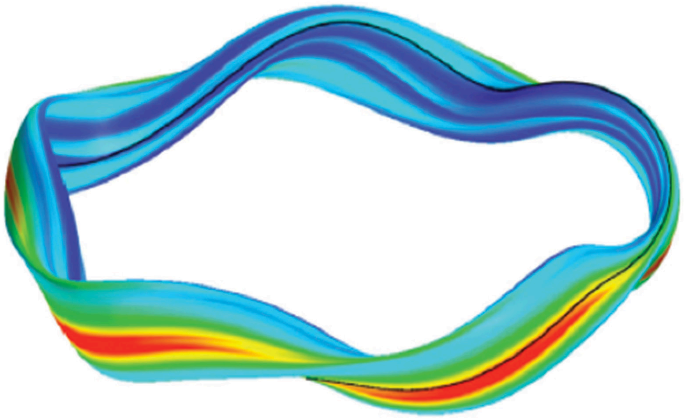
Design optimization

Objective: **Improved Stellarator optimization**

- **Innovations:**

- **Development of computational tools to couple EM GK codes to 3-D (MHD) equilibrium conditions for the purpose of minimizing turbulence to further exploit the optimization potential of stellarators and to determine the effect of the magnetic configuration (3d shaping) on microturbulence.**

- **Development of nonlinear MHD and further development of TRANSP-like transport codes (such as TASK3D) for stellarators . (To properly address the space of configurations)**



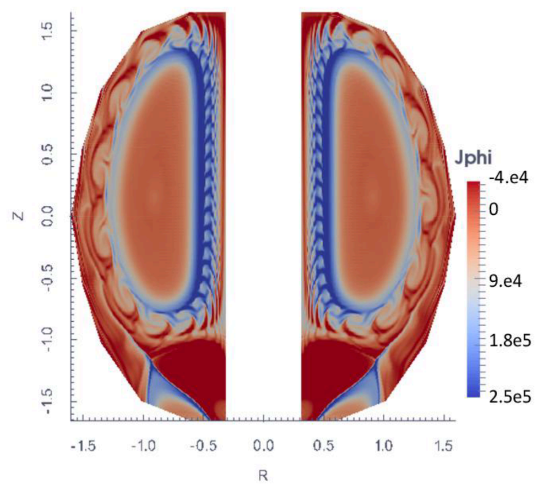
Snapshot of the first full-flux-surface gyrokinetic simulation of plasma turbulence in the Wendelstein 7-X stellarator. (Xanthopoulos et al. 2014)

Design optimization

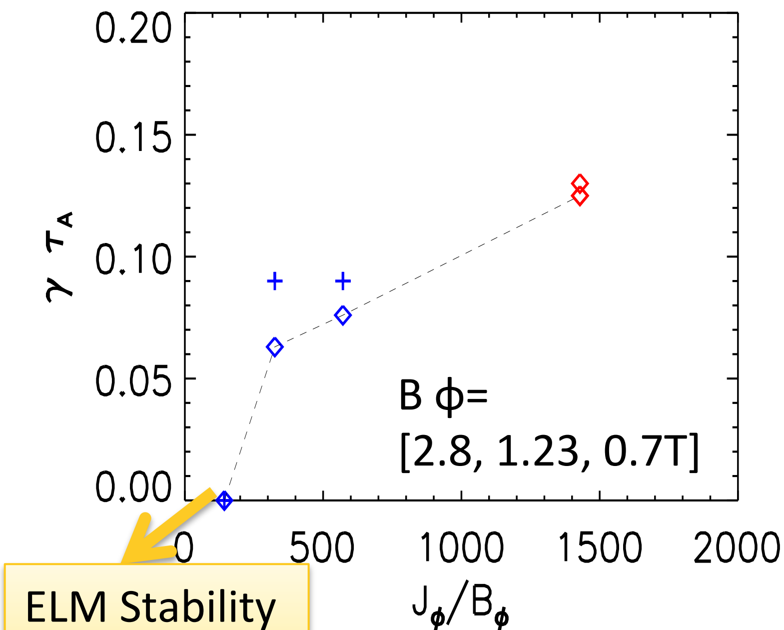
Could HTS suppress/eliminate ELMs?

- Objectives: HTS/high field can be transformative for many different magnetic confinement systems

➢ **Innovations: Theory and simulations to evaluate the implications of HTS on stability and the heat flux width.**



Growth rates of SOL peeling/current-sheet instability



ELM Stability at high field

Simulations with varying Bϕ, but keeping the edge Jϕ = 400kA/m^2 fixed [blue diamond].

Suggesting stability of low-n ELMs in Sts

PoP 24,056119 (2017)

Design optimization

- **Innovations:**

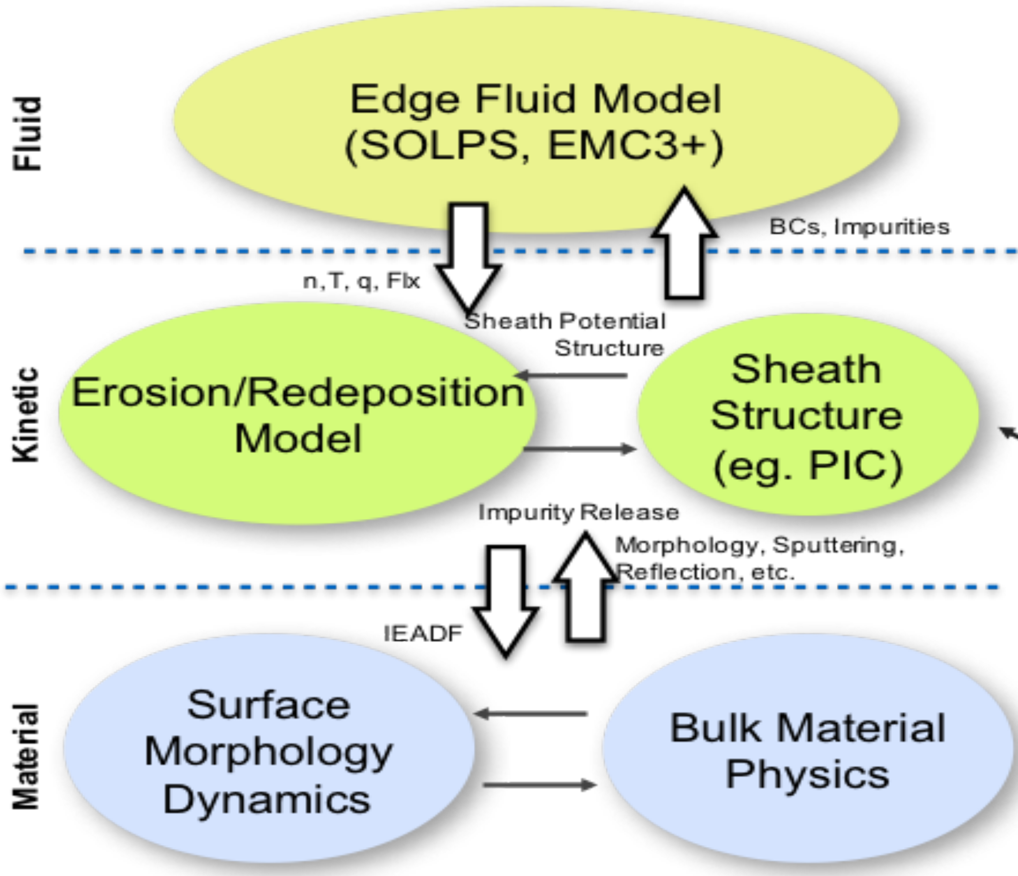
  Compact tokamak/ST design - lower aspect ratio for greater magnetic field utilization, improve stability, reduce TF magnet mass

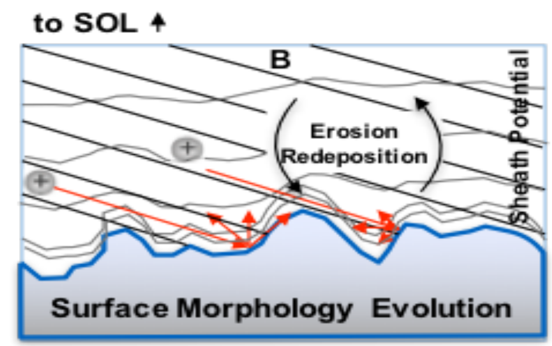
- **Innovations:**

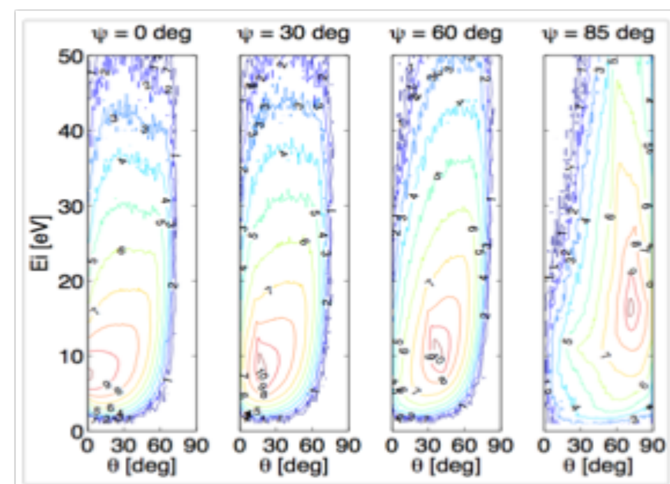
  Integrated physics and engineering optimization design for advanced divertor, blanket, RF launchers, and outside fluid loops is critical for reactor design and safety

Plasma material interface

- **Innovations:**
  - **Multi-scale SOL models include molecular dynamics and kinetic Monte Carlo codes, 2D and 3D plasma transport codes, and 4-5D EM-GK codes**







R.Khaziev, D.Curreli, Phys. Plasmas 22, 043503 (2015)

Summary I

- Computation needs to be reinforced by theory

- **There are approaches to achieve optimization/prediction/control for burning plasmas through WDM**

1. Standalone models
2. Reduced models
3. Integrated modeling through multiphysics-multiscale coupling

- V&V (including experiments via synthetic diagnostic) is required at every level for all approaches

- Whole device modeling, with support from ASCR/ECP, could be game changing for fusion.

Two reports on integrated simulations and exascale:
2015 Bonoli-Curfman Report:
https://science.energy.gov/~/media/fes/pdf/workshop-reports/2016/ISFusionWorkshopReport_11-12-2015.pdf
2016 Chang-Greenwald Report:
http://exascaleage.org/wp-content/uploads/sites/67/2017/06/DOE-ExascaleReport-FES-Final.pdf

Summary II

- In addition to filling the gaps/opportunities for existing fusion experiments, we should be open for theory and computation to guide us to new exciting experiments

- **Theory and computations could have a significant role to promote synergy between fusion program and other branches of plasma physics** research and could further strengthen

  1. US plasma science leadership in the world
  2. The mutual interaction to ensure future innovation
  3. Educational plasma physics environments

Summary III

	Fusion pathways->	Configurations		Technology		Understanding
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Exascale computing – GPU - Advanced numerical algorithms - Deep learning, artificial intelligence

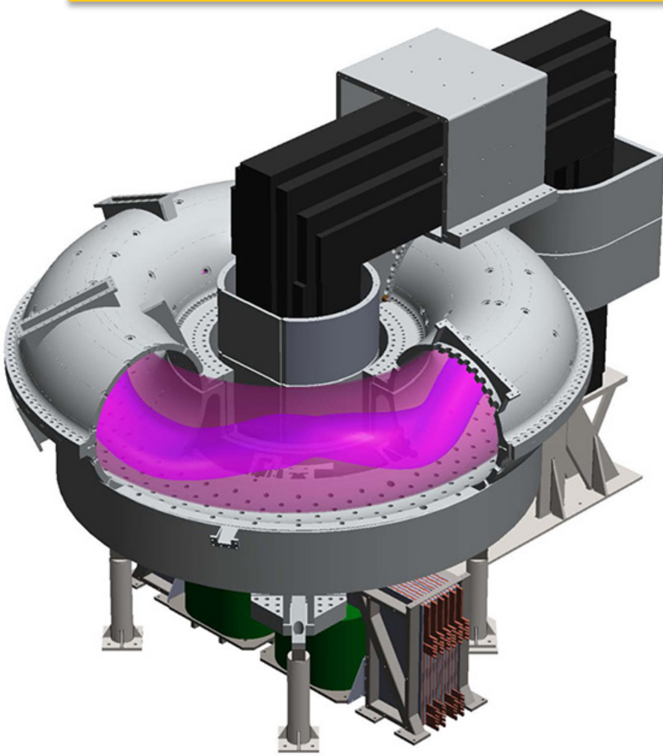
Development of predictive capability for non-inductive current-drive techniques - Improved Stellarator optimization - Integrated Physics and Engineering design

Reliably predict scrape-off layer transport and beyond

Slides on some examples

1- How to validate for multi-scale-multi-physics problems?

- Validation on a device without dominant time/length scale is challenging
- Simpler devices are valuable validation tools, or specific validation experiment should be used



3D helical instability in MST

- Other MFE devices have been successfully used as validation targets
- Other MFEs: FRC, spheromaks,

- For example RFP was used as a validation target using a standalone model (MHD)
- First validation of nonlinear MHD (in early 90's Schnack et al.) done in RFP

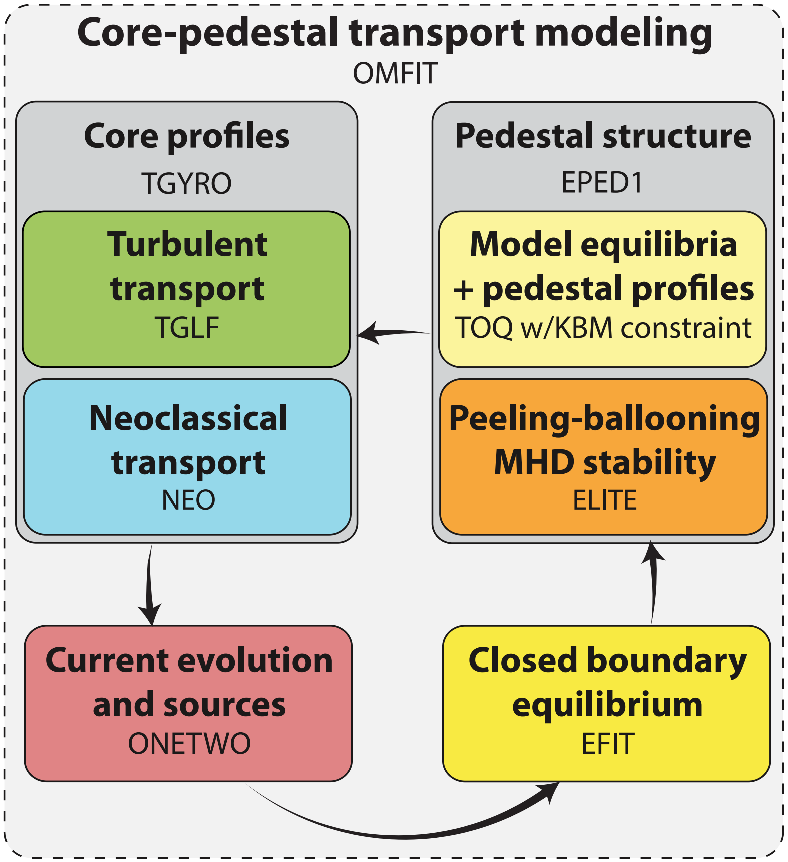
- Even non-MFE devices could play a valuable role for example LAPD (realistic physics parameters and allow further extrapolation)

2- Reduced models in a WDM framework for fast prediction

- Combining core, pedestal and MHD equilibrium solvers the core plasma profiles can be predicted

Verification with HPC simulations and validation with experimental data

➢ AToM will Evolve Towards Whole Device Modeling by Including Boundary Models



3- WDM through integrated coupled models

Types of coupling

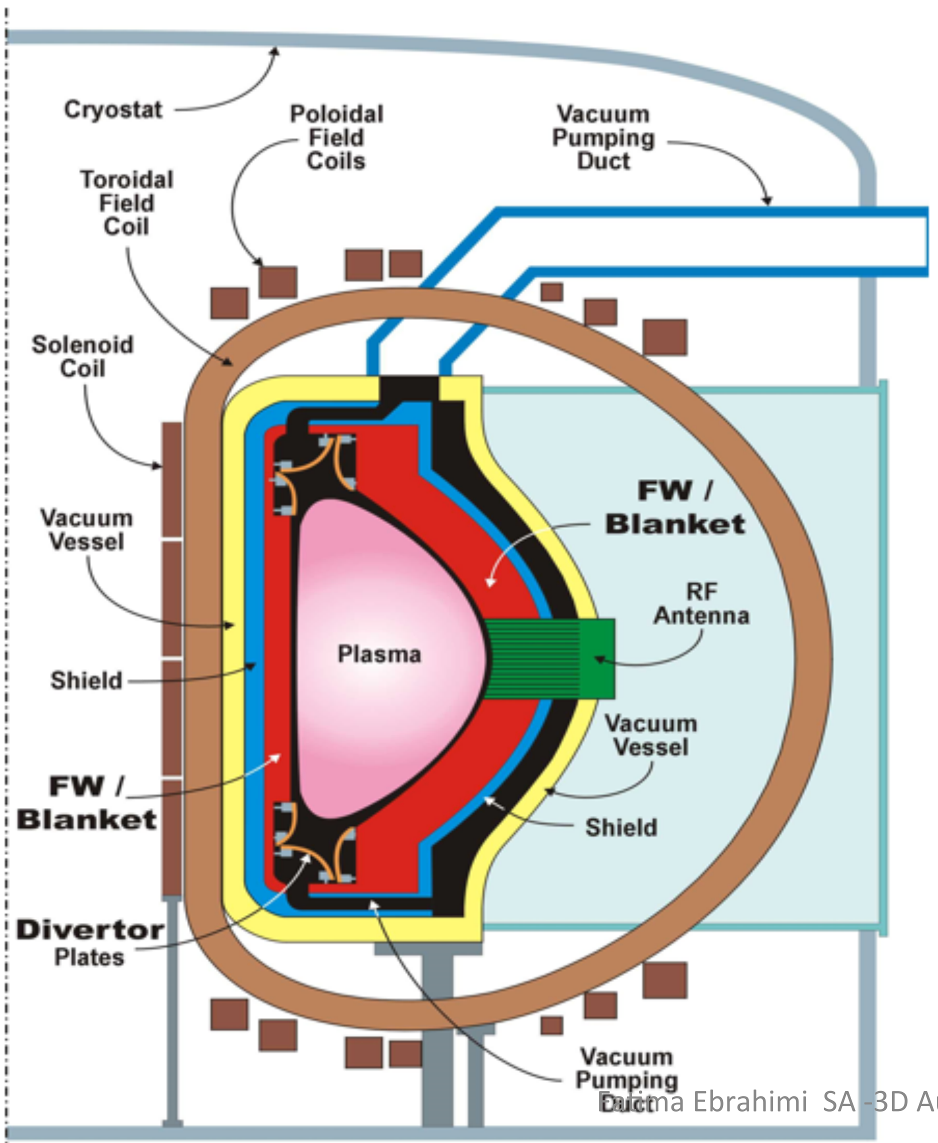
- **RF-MHD**
  - MHD response to RF
- **Kinetic core-edge**
  - Core – Pedestal – SOL using exascale computing
- **MHD – kinetic**
  - stabilizing physics effects- energetic particles - runaway electrons
- **SOL plasma – multi material**
  - coupling EM gyrokinetic to and comprehensive models of neutral particle and radiation transport

Challenges for high-fidelity WDM

- **Implicit time-advance (bridging time-scales)**
- **Large spans of temporal and spatial scales**
  - Steep edge gradients, large range of timescales
  - require high order spatial/temporal algorithms
- **Continuity of solutions across separatrix**
- **Noise-reduction techniques**
- **Input uncertainties**
  - Verification, validation with UQ
- **Synthetic diagnostics and data management**

- **Mathematical and computational technologies will be needed**
- WDM = Fusion + Computer science +Applied Math
- **Inclusion of advanced solver/iteration algorithms**

Core burning plasma is connected to external systems



- **Plasma edge:** is of the greatest importance as it is coupled to the core temperature and density on one hand, and on the other hand it determines wall heat loads and material erosion.

- **Wall/ antennas**

Core plasma models should be coupled to all the external systems

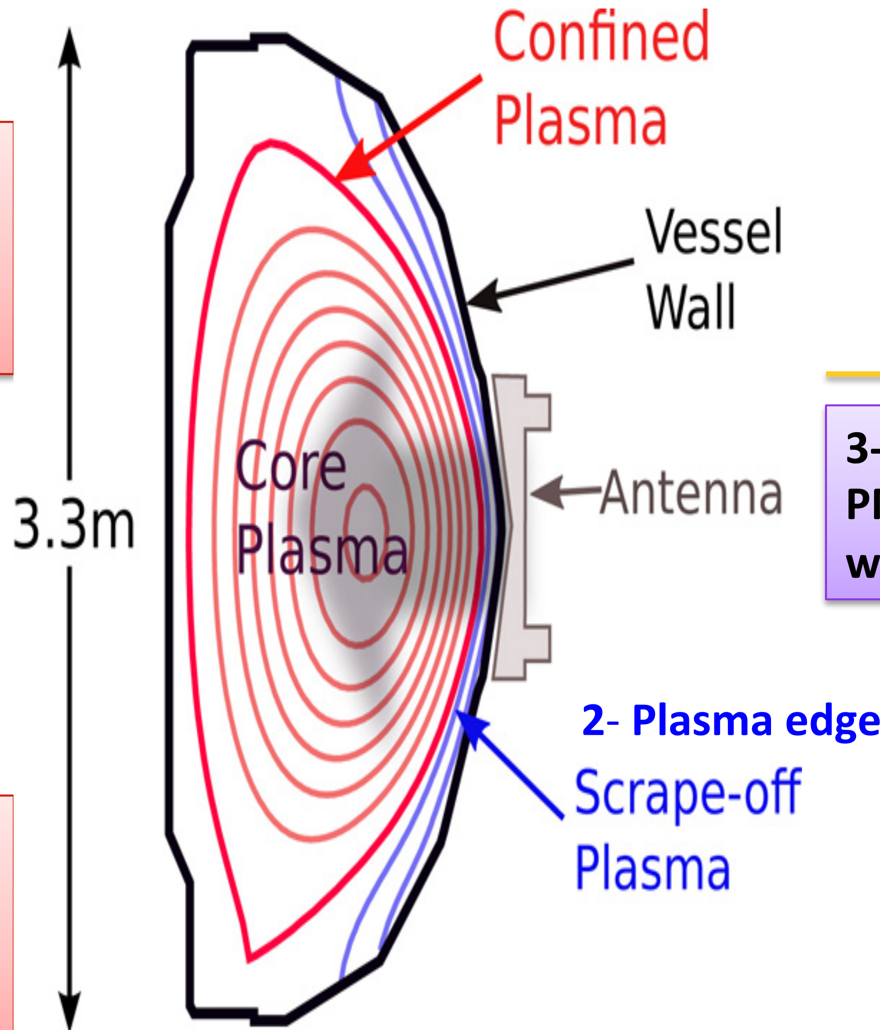
1- Core plasma

Core turbulent/
neoclassical
transport
Kinetic approach

reconnection

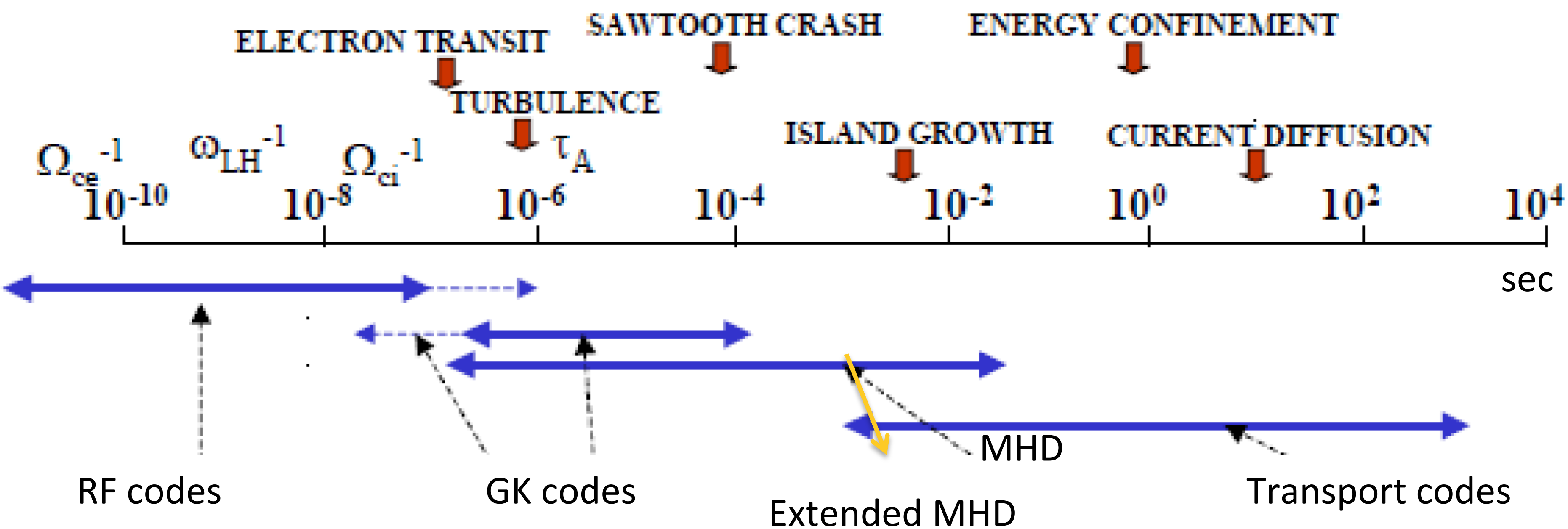
Turbulence

Fluid approach
MHD
Macroscopic
stability



3- Fusion specific:
PMI –RF antennas –
wall, beams

There are enormous multi-scale challenges for modeling burning tokamak plasma



Need to take into account all the physics models and the external systems

- **High fidelity models:**
  - RF, Extended MHD, Gyro-fluid, Gyrokinetic , 3D PIC, 6D Vlasov (standalone models may have some weak coupling)

- **Integrated coupled models - types of coupling:**
  - **RF-MHD**
    - MHD response to RF
  - **Kinetic core-edge**
    - Core – Pedestal - SOL coupling through gyrokinetic core-edge coupling using exascale computing
  - **MHD – kinetic**
    - stabilizing physics effects - energetic particles - runaway electrons
  - **SOL plasma – multi material**
    - coupling EM gyrokinetic to comprehensive models of neutral particle and radiation transport

- **Neural network: Machine learning to create faster reduced models** –

NN uses an algorithm to assign values to a set of weighting parameters to reproduce a known output for a given input data set. If the NN is successfully trained based on full physics models, it will produce reasonable output also for other, similar input data.

Innovations, cont.

- Applications of advanced numerical algorithms, e.g., for
  - large-scale non-linear and linear solvers
  - implicit, IMEX, and simplectic integrators for time advance
  - high-order finite-volume, discontinuous Galerkin, etc., discretizations on mapped/singular grids
  - stable coupling algorithms for stiff components
  - noise control and minimization

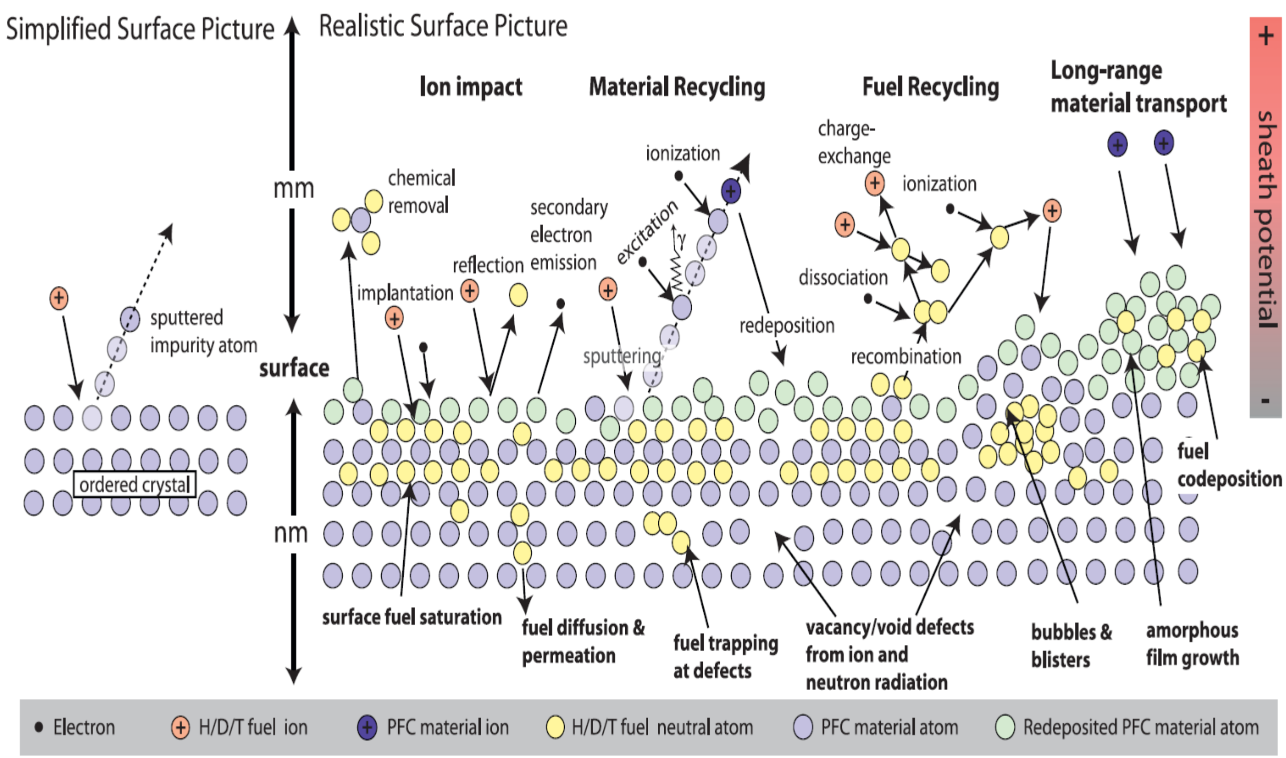
Much (not all) of our algorithm development is carried out under SciDAC; some is under the ECP:

- approaches known to or developed by ASCR partners, brought to MFE
- approaches developed in ASCR/MFE collaboration

From L. Lodestro

Plasma material interface

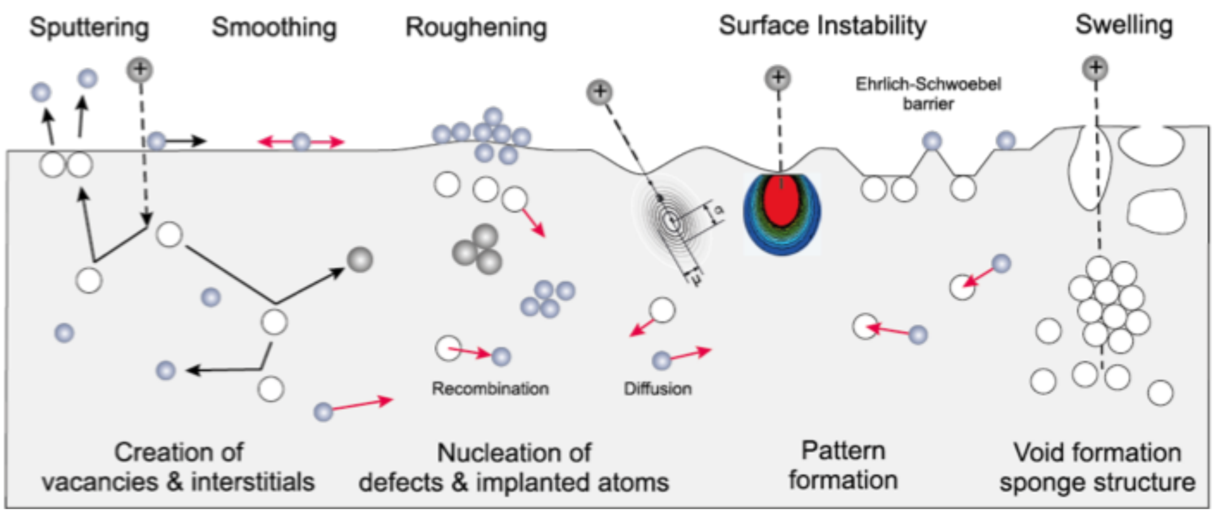
- **Innovations: Develop an enhanced capability to couple wall response models to plasma models. A related activity is to examine advanced divertor concepts, including alternate magnetic-geometry divertors and liquid walls.**
  - **Multi-scale SOL models include molecular dynamics and kinetic Monte Carlo codes, 2D and 3D plasma transport codes, and 4-5D EM-GK codes**
  - Especially important for coupling are efficient wall models for erosion / redeposition of surfaces, impurity release, and tritium trapping within the wall

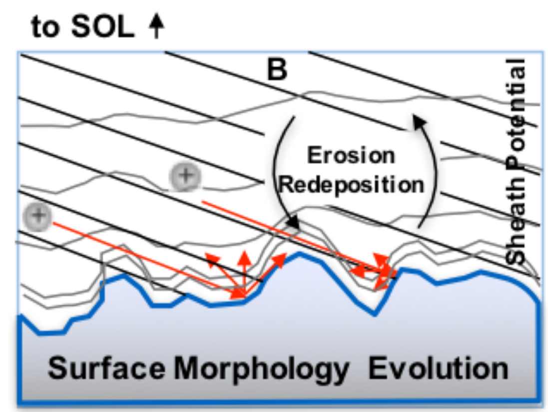


Comparison of a simplified plasma/surface model where only sputtering occurs (left) with a realistic model (right) where many types of interactions occur within the material during bombardment by a fusion plasma. Image courtesy of B. Wirth.

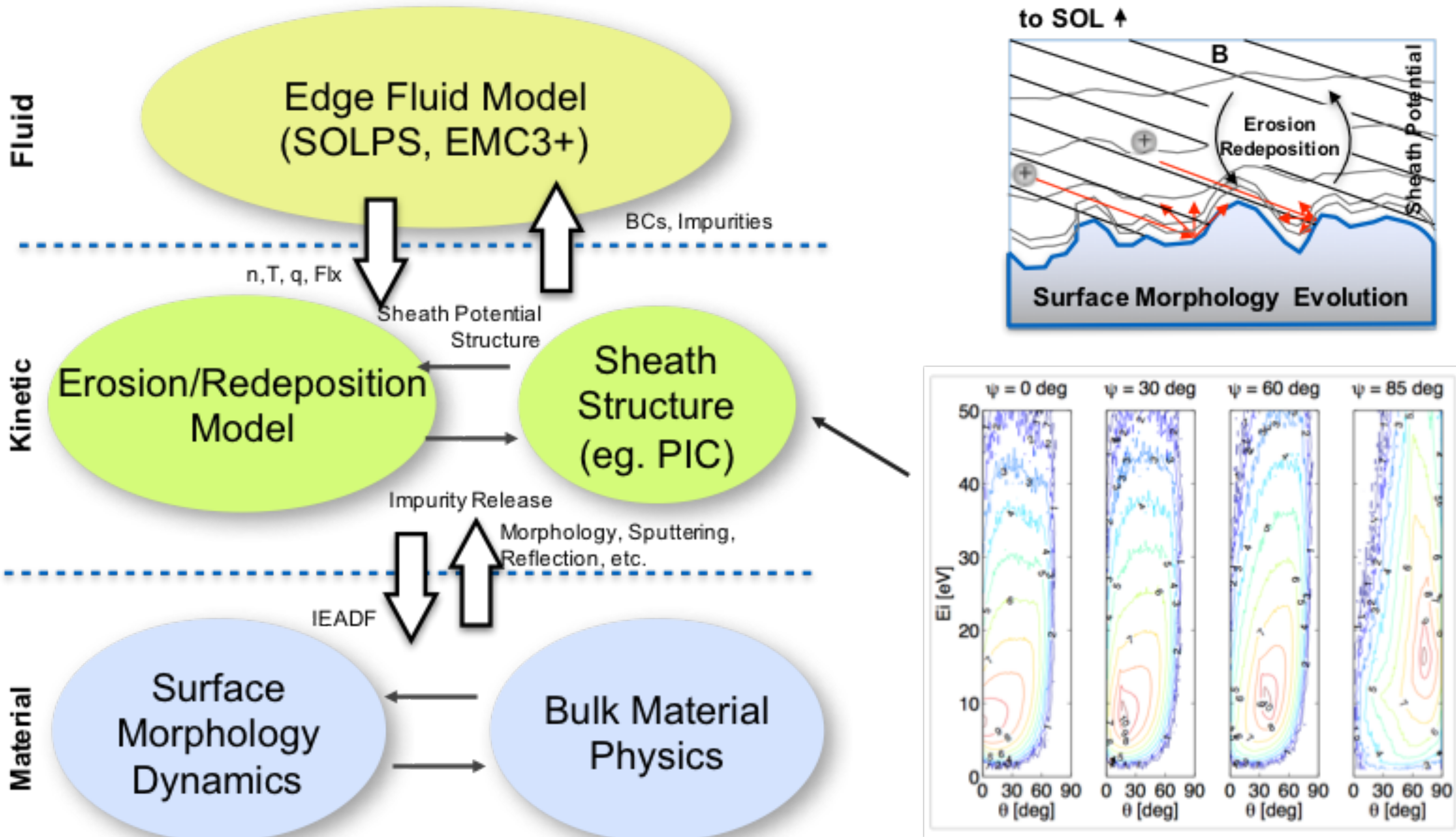
AN *INCOMPLETE* LIST OF BIG UNKWNOWNS

- **Basic understanding**:
  1. effects of the PMI in the plasma core,
  2. understanding of the plasma-material system intended as a dynamically-coupled system,
  3. intermediate steps uncertain between erosion and core plasma
  4. Surface layers of PFM are rapidly and continually being reconstituted by plasma erosion and re-deposition: how the material surface evolves on "mesoscopic" time scales (multiple diff times)
- **Diagnosis**: the complexity of the extreme PSI environment requires a more complex set of characterization tools that must probe dynamically ultra-shallow regions





Systematic approach at multi-scale physics of the material and plasma interaction

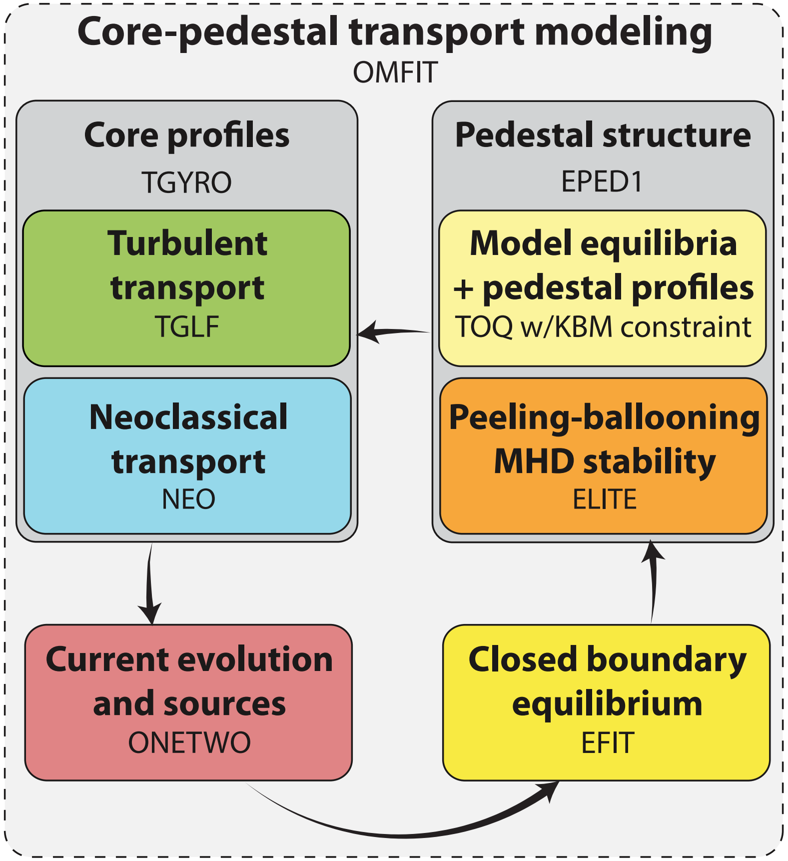


R.Khaziev, D.Curreli, Phys. Plasmas 22, 043503 (2015)

OMFIT Managed Core-Pedestal Modeling is a Prototype Predictive Modeling Workflow

- **Combining core, pedestal and MHD equilibrium solvers the core plasma profiles can be predicted**
  - Predicted profiles can be easily verified with HPC simulation codes

- **The next step is to use the predicted profiles for simulation of diagnostic signals for DIII-D**
  - MHD, TAE, NTM, KBM, EHO, PBM
  - Turbulence spectra: ITG, TEM, ETG
  - Fast ion losses and profiles
  - Impurity transport and radiation
  - All DIII-D diagnostic modules



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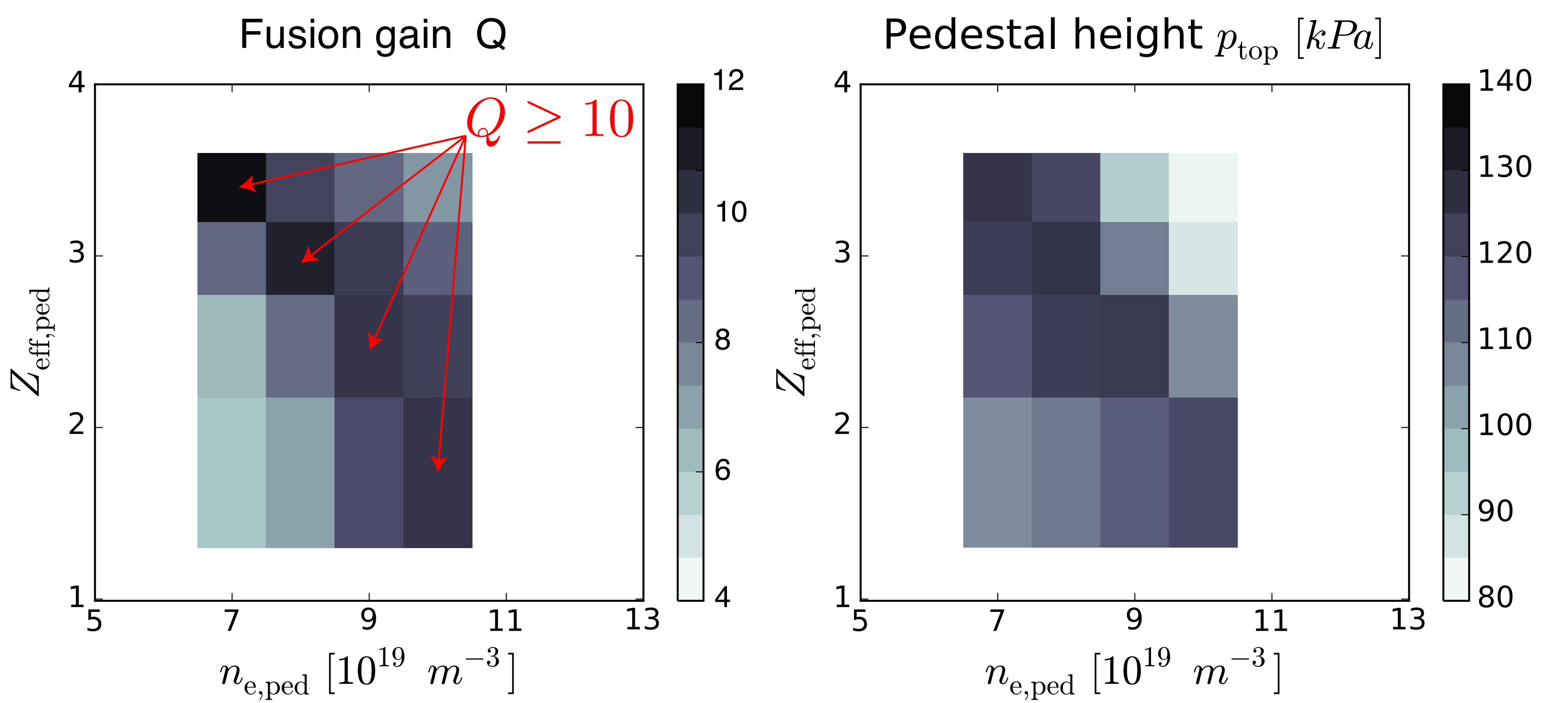
OMFIT Managed Core-Pedestal Modeling Predicts ITER Optimization

- **The OMFIT managed integrated core transport workflow using predicts Q=10 for ITER inductive H-mode for an optimized pedestal density**
- **The highest Q follows the pedestal pressure maximum due to the bootstrap current impact on ELM stability**



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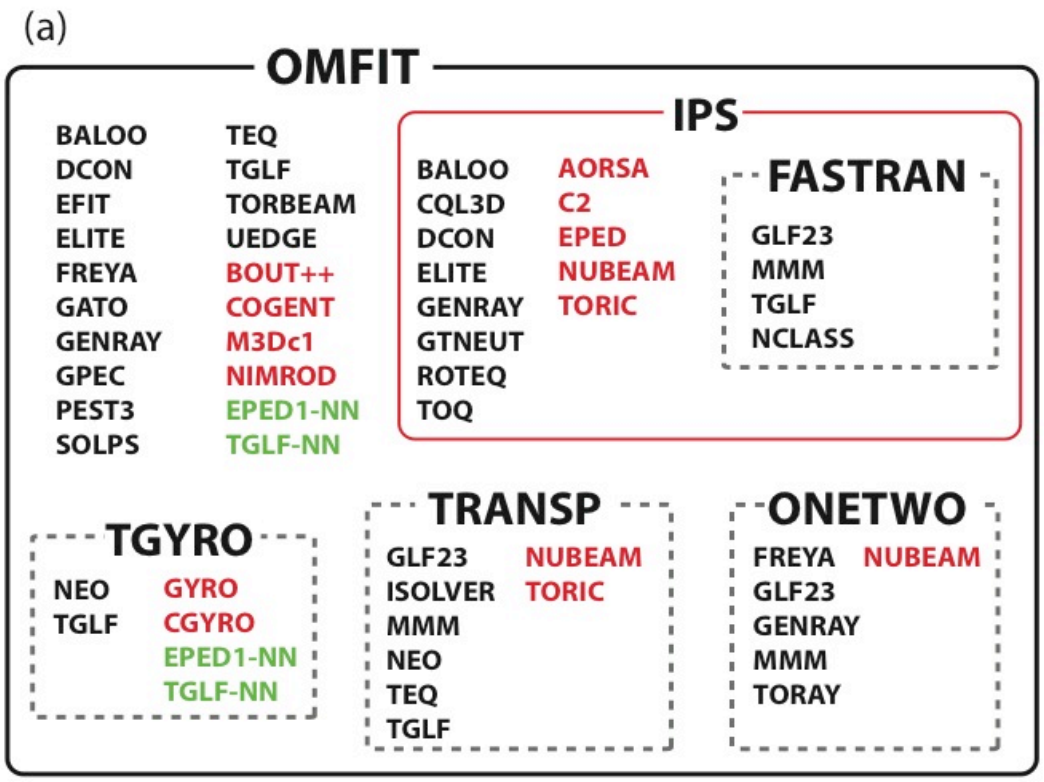
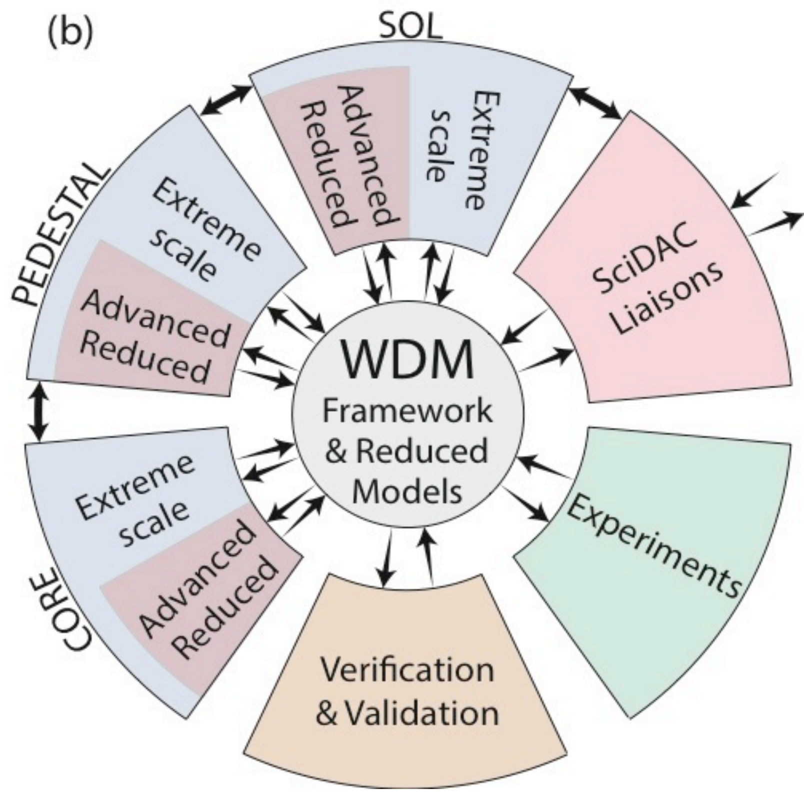
AToM will Evolve Towards Whole Device Modeling by Including Boundary Models

- **Boundary physics codes will be coupled to pedestal and core codes**
  - UEDGE, SOLPS, BOUT++, COGENT …
- **Reduced models in a WDM framework for fast prediction**
- **Verification with HPC simulations and validation with experimental data**





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Plasma Physics - core to edge

Predictive integrated modeling

- Objective: Reliably **predict disruption scenarios** from instability to final wall deposition

➢ **Innovations: Development of theory, extended MHD (core to edge), and reduced models coupled to real-time forecasting**

- Objective: Reliably predict MHD equilibrium **for H-mode perform**ance by understanding pedestal structure, MHD stability, turbulence, and nonlinear/neoclassical transport across entire ELM cycle including SOL transport and divertor heat load width

➢ **Innovations: Core − Pedestal - SOL coupling through gyrokinetic core-edge coupling using exascale computing / First principles 6D Vlasov codes using extreme scale computers**

- Objective: Reliably **predict scrape-off layer transport and beyond**

➢ **Innovations: coupling EM gyrokinetic to comprehensive models of neutral particle and radiation transport, to multi-species plasma sheath mode and to a multi-scale material model using exascale platform**